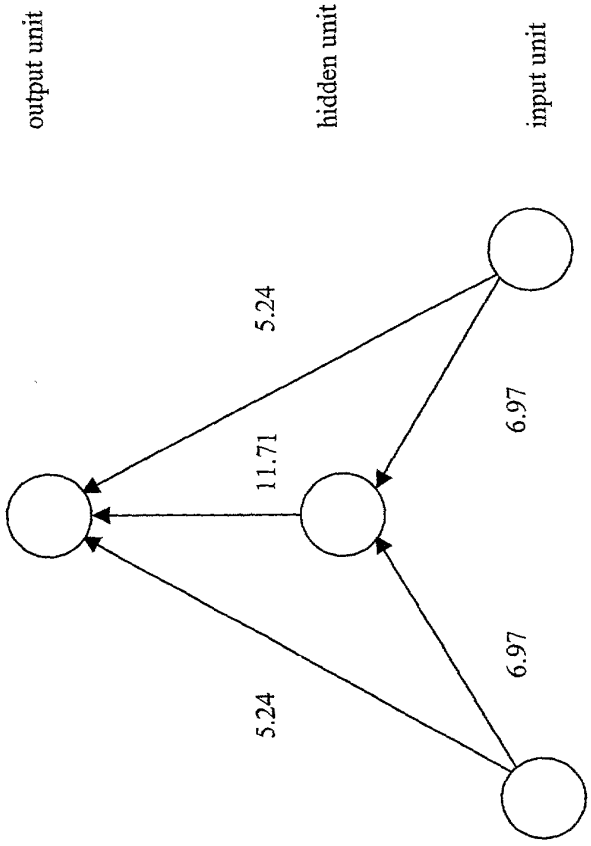

Figure 1

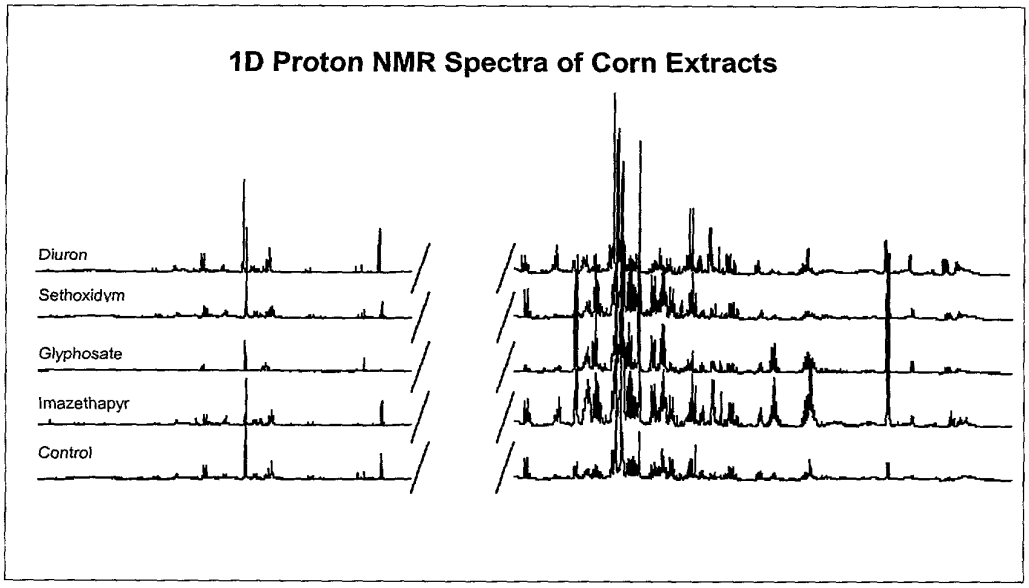

Figure 2

EFS Web - PRINT

Batch_Spectrum	Seq. No.	Treatment	NetworkOutput: Node/Node Value						Network Output
Training Set			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na022400_02	2	Control	0.99996	0	0.00001	0.00003	0.00002	0.00001	Control
na022400_05	5	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_06	29	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_09	32	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
na030100_11	**34**	**PURSUIT**	**0**	**0.99996**	**0.00001**	**0.00003**	**0.00004**	**0.00002**	**PURSUIT**
na030100_14	**37**	**PURSUIT**	**0**	**0.99996**	**0.00001**	**0.00004**	**0.00004**	**0.00002**	**PURSUIT**
na030100_17	**40**	**PURSUIT**	**0**	**0.99995**	**0.00002**	**0.00003**	**0.00004**	**0.00002**	**PURSUIT**
na030100_19	**42**	**PURSUIT**	**0**	**0.99995**	**0.00001**	**0.00004**	**0.00004**	**0.00002**	**PURSUIT**
na030600_04	51	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	55	Sethoxydim	0.00002	0.00001	0.99996	0.00005	0.00001	0.00004	Sethoxydim
na030600_10	57	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
na030600_13	60	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
na030600_15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
na030600_16	63	Glyphosate	0.00006	0.00004	0.00003	0.99994	0	0.00003	Glyphosate
na030600_20	67	Diuron	0.00004	0.00004	0.00002	0	0.99993	0.00003	Diuron
na030600_21	68	Diuron	0.00007	0.00004	0 00002	0	0.99994	0.00003	Diuron
Test Set									
na022400_01	1	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na022400_03	3	Control	0.99996	0	0.00001	0.0001	0.00002	0.00001	Control
na022400_04	4	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na022400_06	6	Control	0.99997	0	0.00002	0	0	0	Control
na022400_07	7	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na022400_08	8	Control	0.99997	0	0.00001	0.00001	0.00001	0.00001	Control
na022400_09	**9**	**PURSUIT**	**0**	**0.02733**	**0**	**0.01224**	**0**	**0.00006**	**Unknown**
na022400_10	**10**	**PURSUIT**	**0.00086**	**0.00118**	**0**	**0.34361**	**0**	**0.00002**	**Unknown**
na022400_11	**11**	**PURSUIT**	**0.00085**	**0.00141**	**0**	**0.27197**	**0**	**0.00002**	**Unknown**
na022400_12	**12**	**PURSUIT**	**0.00016**	**0.0025**	**0**	**0.12513**	**0**	**0.00003**	**Unknown**
na022400_13	**13**	**PURSUIT**	**0.00013**	**0.00259**	**0**	**0.12979**	**0**	**0.00003**	**Unknown**
na022400_14	**14**	**PURSUIT**	**0.00013**	**0.00238**	**0**	**0.13242**	**0**	**0.00003**	**Unknown**
na022400_15	**15**	**PURSUIT**	**0**	**0.10029**	**0**	**0.00586**	**0.00001**	**0.0001**	**Unknown**
na022400_16	**16**	**PURSUIT**	**0.00005**	**0.00469**	**0**	**0.06222**	**0**	**0.00004**	**Unknown**
na022400_17	**17**	**PURSUIT**	**0.00114**	**0.00127**	**0**	**0.29608**	**0**	**0.00002**	**Unknown**
na022400_18	**18**	**PURSUIT**	**0.00091**	**0.00139**	**0**	**0.27092**	**0**	**0.00002**	**Unknown**
na022400_19	**19**	**PURSUIT**	**0.00048**	**0.00185**	**0**	**0.18992**	**0**	**0.00002**	**Unknown**
na022400_20	**20**	**PURSUIT**	**0.00214**	**0.00104**	**0**	**0.35051**	**0**	**0.00002**	**Unknown**
na022400_21	**21**	**PURSUIT**	**0.00073**	**0.00088**	**0**	**0.34762**	**0**	**0.00002**	**Unknown**
na022400_22	**22**	**PURSUIT**	**0.00046**	**0.00146**	**0**	**0.25479**	**0**	**0.00002**	**Unknown**
na022400_23	**23**	**PURSUIT**	**0.00086**	**0.00123**	**0**	**0.3072**	**0**	**0.00002**	**Unknown**
na030100_01	24	Control	0.99996	0	0	0.00002	0.00005	0.00001	Control
na030100_02	25	Control	0.99997	0	0	0.00001	0.00238	0.00001	Control
na030100_03	26	Control	0.99997	0	0	0.00001	0.00006	0.00001	Control
na030100_04	27	Control	0.99996	0	0.00002	0	0.00001	0	Control
na030100_05	28	Control	0.99993	0	0.00001	0	0.00002	0.00001	Control

Figure 3a

20070 5795007

Training Set			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na030100_07	30	Control	0.99998	0	0	0.00002	0.00002	0.00001	Control
na030100_08	31	Control	0.99996	0	0.00002	0	0.00001	0.00001	Control
na030100_10	33	PURSUIT	0	0.99996	0.00001	0.00003	0.00005	0.00002	PURSUIT
na030100_12	35	PURSUIT	0	0.99996	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100_13	36	PURSUIT	0	0.99996	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100_15	38	PURSUIT	0	0.99994	0.00003	0.00003	0.00005	0.00002	PURSUIT
na030100_16	39	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_18	41	PURSUIT	0	0.99995	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100_20	43	PURSUIT	0	0.9999	0.00005	0.00003	0.00008	0.00003	PURSUIT
na030100_21	44	PURSUIT	0	0.99995	0.00004	0.00004	0.00003	0.00002	PURSUIT
na030100_22	45	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030600_12	59	Sethoxydim	0.00005	0.0003	0.99701	0	0.00003	0.00003	Sethoxydim
na030600_14	61	Glyphosate	0.00006	0.00004	0.00002	0.99994	0	0.00003	Glyphosate
na030600_17	64	Glyphosate	0.00005	0.00005	0.00003	0.99993	0	0.00003	Glyphosate
na030600_18	65	Foul	0	0.00007	0.00003	0	0.00001	0.99993	Foul
na030600_19	66	Diuron	0.00034	0.00003	0.00002	0	0.99992	0.00003	Diuron
na030600_22	69	Diuron	0	0.00005	0.00003	0	0.99989	0.00004	Diuron
na030600_23	70	Diuron	0.00065	0.00014	0.00043	0	0.92715	0.00011	Diuron
na030600_24	71	Diuron	0.00002	0.00005	0.00003	0	0.99993	0.00003	Diuron
Training Set									
na022400_02	2	Control	0.99996	0	0.00001	0.00003	0.00002	0.00001	Control
na022400_05	5	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_06	29	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_09	32	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
na030100_11	34	PURSUIT	0	0.99996	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100_14	37	PURSUIT	0	0.99996	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030100_17	40	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_19	42	PURSUIT	0	0.99995	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030600_04	51	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	55	Sethoxydim	0.00002	0.00001	0.99996	0.00005	0.00001	0.00004	Sethoxydim
na030600_10	57	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
na030600_13	60	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
na030600_15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
na030600_16	63	Glyphosate	0.00006	0.00004	0.00003	0.99994	0	0.00003	Glyphosate
na030600_20	67	Diuron	0.00004	0.00004	0.00002	0	0.99993	0.00003	Diuron
na030600_21	68	Diuron	0.00007	0.00004	0.00002	0	0.99994	0.00003	Diuron

Figure 3b

SNNS result file	V1.4-3D					
Training file	na022400					
Test file na040400						
No. of patterns:	24					
No. of input units:	1080					
No. of output units:	6					
Startpattern:	1					
Endpattern:	24					
Teaching output included						
Treatment:	1.1 Control					
Target:	1	0	0	0	0	0
Output:	0.99954	0.00045	0.00001	0.00001	0.00001	0.00001
Treatment:	2.1 Control					
Target:	1	0	0	0	0	0
Output:	0.99936	0.00065	0.00001	0.00001	0.00001	0.00001
Treatment:	3.1 Control					
Target:	1	0	0	0	0	0
Output:	0.99951	0.00047	0.00001	0.00001	0.00001	0.00001
Treatment:	4.1 Control					
Target:	1	0	0	0	0	0
Output:	0.99963	0.00037	0.00001	0.00001	0.00001	0.00001
Treatment:	5.1 Chlorsulfuron					
Target:	0	0	0	0	0	0
Output:	0.00159	0.99843	0	0.00001	0	0
Treatment:	6.1 Chlorsulfuron					
Target:	0	0	0	0	0	0
Output:	0.00806	0.99165	0	0	0	0
Treatment:	7.1 Chlorsulfuron					
Target:	0	0	0	0	0	0
Output:	0.00334	0.99669	0	0	0	0
Treatment:	8.1 Chlorsulfuron					
Target:	0	0	0	0	0	0
Output:	0.00014	0.99985	0	0.00001	0	0
Treatment:	9.1 Chlorsulfuron					
Target:	0	0	0	0	0	0
Output:	0.00667	0.99376	0	0	0	0
Treatment:	10.1 Imazamethabenz					
Target:	0	0	0	0	0	0
Output:	0.00044	0.99955	0	0	0	0
Treatment:	11.1 Imazamethabenz					
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	0	0	0	0
Treatment:	12.1 Imazamethabenz					
Target:	0	0	0	0	0	0
Output:	0.00208	0.99798	0	0.00001	0.00001	0

Figure 4a

SNNS result file	V1.4-3D					
Training file	na022400					
Test file na040400						
No. of patterns:	24					
No. of input units:	1080					
No. of output units:	6					
Startpattern:	1					
Endpattern:	24					
Teaching output included						
Treatment:	13.1 Imazamethabenz					
Target:	0	0	0	0	0	0
Output:	0.00223	0.99755	0	0	0	0
Treatment:	14.1 Imazamethabenz					
Target:	0	0	0	0	0	0
Output:	0.06789	0.93484	0	0	0	0
Treatment:	15.1 Sulfumeturon					
Target:	0	0	0	0	0	0
Output:	0.00046	0.99955	0	0	0	0
Treatment:	16.1 Sulfumeturon					
Target:	0	0	0	0	0	0
Output:	0.00102	0.999	0	0.00001	0	0
Treatment:	17.1 Sulfumeturon					
Target:	0	0	0	0	0	0
Output:	0.00194	0.99813	0	0.00001	0	0
Treatment:	18.1 Sulfumeturon					
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	0	0	0	0
Treatment:	19.1 Sulfumeturon					
Target:	0	0	0	0	0	0
Output:	0.00014	0.99985	0	0	0	0
Treatment:	20.1 Imazapyr					
Target:	0	0	0	0	0	0
Output:	0.0018	0.998	0	0	0	0
Treatment:	21.1 Imazapyr					
Target:	0	0	0	0	0	0
Output:	0.00031	0.99968	0	0.00001	0	0
Treatment:	22.1 Imazapyr					
Target:	0	0	0	0	0	0
Output:	0.00175	0.99791	0	0	0	0
Treatment:	23.1 Imazapyr					
Target:	0	0	0	0	0	0
Output:	0.00018	0.9998	0	0	0	0
Treatment:	24.1 Imazapyr					
Target:	0	0	0	0	0	0
Output:	0.06579	0.93074	0	0	0	0

Figure 4b

20010 Statsoft

Class	Control	AHAS	ACCase	EPSPS	PS II	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin Transp	DHP	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis	Unknown	No Class
Control	54						1					1												3
AHAS		30																						
ACCase			6																					
EPSPS				4																				
PS II					6																			
Necrotic*						2																		
HPPD							10																	2
PROTOX								12																
Carotenoid									12															
PSI										9														3
Microtubule	1										7													4
PDS												5												1
Uncoupler													9											3
Auxin-like														11										1
Auxin Transp															8	1								3
DHP											1					8								3
Acetamide																	6							
PSII_c1																		9						3
PSII_c2																		1	10					1
PSII_c3																				12				
Glutamine																					22			2
Mitosis																						8		4
Unknown																								
NoClass																								

Rows: Teaching Input; Columns: Classification for Nineteen MOAs
(23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 5

CLASS	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin Transp	DHP	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis	Spare	Unknown	# Plants
Control	27	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	2	31
AHAS	0	17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17
ACCase	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3
EPSPS	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
Not Used	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Necrotic*	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
HPPD	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	6
PROTOX	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6
Carotenoid	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6
PSI	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	2	6
Microtubule	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	4	6
PDS	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	2	3
Uncoupler	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	1	0	0	0	0	0	0	0	1	6
Auxin-like	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	2	6
Auxin Transp	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	0	0	0	0	0	0	0	2	6
DHP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	5	6
Acetamide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	1	3
PSII_c1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	0	0	0	0	2	6
PSII_c2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	8	0	0	0	0	1	10
PSII_c3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	6
Glutamine	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	11	0	0	0	12
Mitosis	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	3	6
Spare	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NoClass	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Rows: Teaching Input; Columns: Classifications for Nineteen MOAs
(23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 6

MOA	Control	AHAS	ACCase	EPSPS	PS II	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin Transp	DHP	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis	Spare	Unknown
Control	92						2					2												5.8
AHAS		100																						
ACCase			100																					
EPSPS				100																				
PS II					100																			
Necrotic*						100																		
HPPD							83																	17
PROTOX								100																
Carotenoid									100															
PSI										75														25
Microtubule	8										58													33
PDS												83												17
Uncoupler													75											25
Auxin-like														92										8.3
Auxin Transp															67	8								25
DHP											8					67								25
Acetamide																	100							
PSII_c1																		75						25
PSII_c2																		8	83					8.3
PSII_c3																				100				
Glutamine																					92			8.3
Mitosis																						67		33

*Necrotic = dead or decaying plant

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 7

Applicant: Arambar et al
Serial No: Filed Concurrently Herewith
Title: Metabolome Profiling Methods Using Chromatographic and Spectroscopic Data in Pattern Recognition Analysis
Docket No. 16513-0089

CLASS	Class	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin Transp	DHP	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis	Spare	Unknown
Control	0	87						3					3												6
AHAS	1		100																						
ACCase	2			100																					
EPSPS	3				100																				
Not Used	4																								
Necrotic*	5						100																		
HPPD	6							50																	50
PROTOX	7								100																
Carotenoid	8									100															
PSI	9										67														33
Microtubule	10											33													67
PDS	11												33												67
Uncoupler	12													67			17								17
Auxin-like	13														67										33
Auxin Transp	14															50	17								33
DHP	15																17								83
Acetamide	16																	67							33
PSII_c1	17																		50	17					33
PSII_c2	18																		10	8					10
PSII_c3	19																				100				
Glutamine	20	8																				92			
Mitosis	21																						50		50

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs
(23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 8